Investigation of Compression Behavior of Heusler Compounds Using Various Equations of State

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Abstract

The compression behaviour of Heusler compounds viz, Rh_2MnZn, Rh_2FeZn, Co_2NbB, and Co_2TaB has been studied using various equations of state, namely Tait equation, Murnaghan equation, Shanker's equation and Kholiya and Chandra equation. It has been observed that the Tait equation of state generally fits best for the compression behaviour of the chosen materials, followed by the Murnaghan equation of state, whereas Kholiya and Chandra, and Shanker's equations of state are less accurate. All Heusler compounds exhibit similar patterns in compression behaviour with decreasing volume and increasing pressure with a slight deviation that may be due to their crystal structure and chemical composition. The obtained results are found to be in good agreement with the available experimental values. The results of this study can provide valuable insights into the compressibility and mechanical properties of Heusler compounds, which can inform their potential applications in various fields, including energy harvesting, spintronics, and thermoelectric devices.

1. Introduction

Intermetallic Heusler compounds have attracted significant attention in recent years due to their unique physical, electrical, and magnetic properties. Understanding the compression behaviour of these compounds is crucial for predicting their mechanical properties and for potential applications in fields such as energy storage, thermos-electrics, and spintronics. In this context, several studies have investigated the compression behaviour of different Heusler compounds using various equation of state (EOS) models. In recent days, various multi-component mixture compounds like Mn_2CoCr, Mn_2PtCo, Rh_2MnZn, and Rh_2FeZn are gaining more attention due to their extraordinary properties like compressible and structural properties by changing the pressure, volume and temperature [1-6]. These Heusler compounds are known for their exciting magnetic, electronic, and thermoelectric properties, making them capable materials for various technological applications [7-13]. Heusler compounds have various potential applications due to their unique combination of physical and chemical properties. Some of the major technological applications of such

compounds namely Mn_2CoCr, Mn_2PtCo, Rh_2MnZn, Rh_2FeZn, Co_2NbB and Co_2TaB include:

i. *Magnetic materials:* Heusler compounds reveal high magnetic properties, making them suitable for use in various magnetic applications, such as magnetic storage devices and magnetic sensors.

ii. *Hard Materials:* Heusler compounds exhibit high hardness and wear resistance, making them appropriate for use as hard materials in wear-resistant coatings,

iii. *Energy Storage devices:* All under study Heusler compounds exhibit good electrochemical performance, making them potential materials for use in energy storage devices such as batteries.

iv. *Spintronics:* These materials have been studied for their potential in spintronics, a field that uses the spin of electrons in a solid-state system.

It is worth mentioning that these compounds have a distinctive crystal structure, with alternating layers of transition metal and main group elements, and exhibit a range of magnetic and electronic phases. Because of high thermal stability, these compounds are applicable for high-temperature applications.

The equation of state is a relationship that describes the state of a system in terms of its variables, such as temperature, pressure, volume, and density [14-17]. It is used to predict the behaviour of a substance under different conditions, viz. pressure, volume and temperature, for both systems of a pure component and also for the multi-component mixture. The equations of state are useful in describing the stability of solid material by changing various parameters like pressure, volume entropy and temperature [18-19]. So, the equation of state is a basic characteristic of a matter which makes possible the application of all the general principles of thermodynamics and reflects atomic structure, chemical bonding and stability of material [20-22].

In this paper, we have studied the compressional behaviour of some Co, Rh, Mn based Heusler compounds in terms of calculated values of relative change in volume (V/V_0) and bulk modulus as a function of pressure at constant temperature by using some theoretical models, known as equations of state.

2. Methods of Analysis:

In this study, various equations of state (EOS) have been used to determine the compressional behaviour of Heusler compounds based on Co, Rh, and Mn. This was done by calculating the relative change in volume (V/Vo) and bulk modulus as a function of pressure at a constant temperature. Bulk modulus measures the resistance of a material to change in volume when subjected to external pressure and is determined by the ratio of the infinitesimal change in pressure to the corresponding fractional change in volume. In the present study, we have used Tait equation state, Murnaghan EOS, Kohliya and Chandra and Shanker's equation of state to determine the pressure dependence of volume compression and bulk modulus of some Heusler compounds, namely Mn_2CoCr, Mn_2PtCo, Rh_2MnZn, Rh_2FeZn, Co_2NbB and Co_2TaB.

Tait's equation of state generally fits best for the compression behaviour of the chosen material had given by P.G. Tait in 1888, which was the non-linear relation of compression with pressure for liquids. After many modifications, the new modified form of the equation of state is introduced, known as the Usual Tait equation (UTE) is in the following form for different solids.

$$\frac{V}{V_0} = \left[1 - \frac{1}{B_0+1}\ln\left\{1 + \left(\frac{B_0+1}{B_0}\right)P\right\}\right]$$

Using this realistic approach, we can calculate the relative compression V/V_0 for different solids.

Also, the expression for isothermal bulk modulus $B(P)$by using relation can be written as:

$$B = B_0\frac{V}{V_0}\left\{1 + \left(\frac{B_0+1}{B_0}\right)P\right\}$$

or $$1 + \left(\frac{B_0+1}{B_0}\right)P = \exp\left\{\left(1 - \frac{V}{V_0}\right)(B_0 + 1)\right\}$$

From the above equations, we get

$$B(P) = B_0\frac{V}{V_0}\exp\left\{\left(1 - \frac{V}{V_0}\right)(B_0 + 1)\right\} \quad \dots (1)$$

Which is the Tiat equation for isothermal bulk modulus.

Other equations of states, Murnaghan equation of state, Kholiya and Chandra's equation of state and Shanker's equation of state, are given by the following relations:

Murnaghan EOS [23-25, 32-33] is given by the relation

$$P = \frac{B_0}{B_0'}\left[\exp\left\{-B_0'\ln\left(\frac{V}{V_0}\right)\right\} - 1\right] \quad \dots (2)$$

Kohliya and Chandra's [23-25, 31-35] equation of state is given the relation

$$P = \frac{B_0}{2}\left[(B_0' - 3) - 2(B_0' - 2)\left(\frac{V}{V_0}\right)^{-1} + (B_0' - 1)\left(\frac{V}{V_0}\right)^{-2}\right] \quad \dots (3)$$

Shanker's equation of state [23-25, 32-35] is given by the equation

$$P = B_0\left[\left(1 - \frac{V}{V_0}\right) + \left(B_0' + \frac{1}{2}\right)\left(1 - \left(\frac{V}{V_0}\right)^2\right)\right] \quad \dots (4)$$

3. Result and Discussion:

Heusler compounds are famous for their applications, such as magnetic storage devices. It becomes important to understand their behaviour under various thermodynamic variables. In this study, we have calculated the thermodynamic variable like bulk modulus and its first pressure derivatives by using various equations of states. The input data of Co, Rh, Mn based Heusler compounds required for the present work to calculate the volume compression of six full Heusler compounds are given in Table 1.

Table 1: Input data of Co, Rh, Mn based Heusler compounds

Compounds	B_0 (GPa)	B'_0(GPa)
Mn_2CoCr	171	5.91
Mn_2PtCo	185.6	4.1
Rh_2MnZn	183.2	5.5
Rh_2FeZn	196.9	4.72
Co_2NbB	244.35	3.76
Co_2TaB	241.80	4

Table 2 shows the compression behaviour of Mn_2CoCr at different pressures (in GPa) as predicted by different equations of state: Tait, Murnaghan, Kholiya and Chandra, and Shankers. The V/V_0 values in the table represent the volume of the material at each pressure relative to its initial volume (V_0).

The Tait equation of state predicts that the material's volume decreases gradually with increasing pressure, with a V/V_0 value of 0.9228 at 16 GPa. The Murnaghan equation of state also predicts a similar trend but with a slightly higher V/V_0 value of 0.9251 at 16 GPa. The Kholiya and Chandra equation of state predicts a more rapid decrease in volume, with a V/V_0 value of 0.9272 at 16 GPa. The Shankers equation of state predicts the most rapid decrease in volume, with a V/V_0 value of 0.9283 at 16 GPa (Fig. 1). Overall, the table shows that as the pressure increases, the volume of Mn_2CoCr decreases, which is expected for most materials. However, the exact rate of compression varies depending on the equation of state used to model the behaviour.

Table 2: Compression behaviour of Mn_2CoCr predicted by various EOS

Pressure (GPa)	**Tait Equation of State**	**Murnaghan Equation of State**	**Kholiya and Chandra Equation of State**	**Shankers Equation of State**
	V/V_0	V/V_0	V/V_0	V/V_0
0	1	1	1	1
2	0.99	0.991	0.992	0.9921
4	0.98	0.981	0.982	0.983
6	0.97	0.972	0.9739	0.975
8	0.96	0.961	0.9631	0.9661
10	0.95	0.952	0.954	0.955
12	0.94	0.942	0.9437	0.9438
14	0.931	0.932	0.935	0.936

16	0.9228	0.9251	0.9272	0.9283

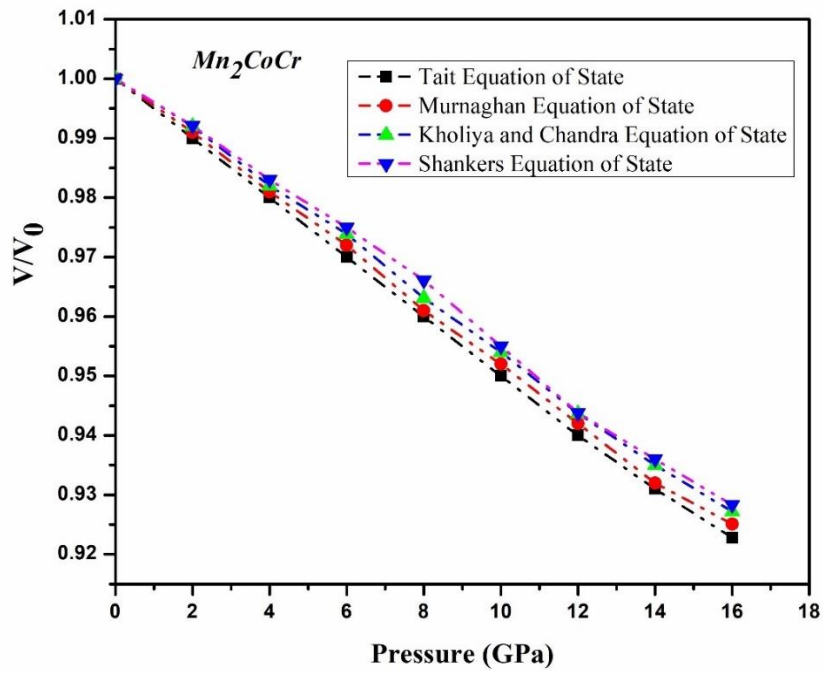

Fig 1. Volume compression with respect to Pressure for Mn_2CoCr

Table 3 shows the compression behaviour of Mn_2PtCo at different pressures (in GPa) as predicted by different equations of state: Tait, Murnaghan, Kholiya and Chandra, and Shankers (shown in Fig 2). The V/V_0 values in the table represent the volume of the material at each pressure relative to its initial volume (V_0). The table shows that as the pressure increases, the volume of Mn_2PtCo decreases, which is consistent with the behaviour of most materials under compression. The Tait equation of state predicts a gradual decrease in volume, with a V/V_0 value of 0.9209 at 16 GPa. The Murnaghan equation of state also predicts a gradual decline in volume, with a slightly higher V/V_0 value of 0.9239 at 16 GPa. The Kholiya and Chandra equation of state predicts a slightly more rapid decrease in volume, with a V/V0 value of 0.925 at 16 GPa. The Shankers equation of state predicts the most rapid reduction in volume, with a V/V_0 value of 0.9258 at 16 GPa.

Table 3: Compression behaviour of Mn_2PtCo predicted by various EOS

Pressure (GPa)	**Tait Equation of State**	**Murnaghan Equation of State**	**Kholiya and Chandra Equation of State**	**Shankers Equation of State**
	V/V_0	V/V_0	V/V_0	V/V_0
0	1	1	1	1
2	0.99	0.992	0.9923	0.9933

4	0.98	0.9815	0.9821	0.9841
6	0.97	0.971	0.9732	0.974
8	0.96	0.961	0.9625	0.9642
10	0.95	0.9513	0.9521	0.9544
12	0.94	0.942	0.9431	0.9415
14	0.93	0.9315	0.9325	0.9331
16	0.9209	0.9239	0.925	0.9258

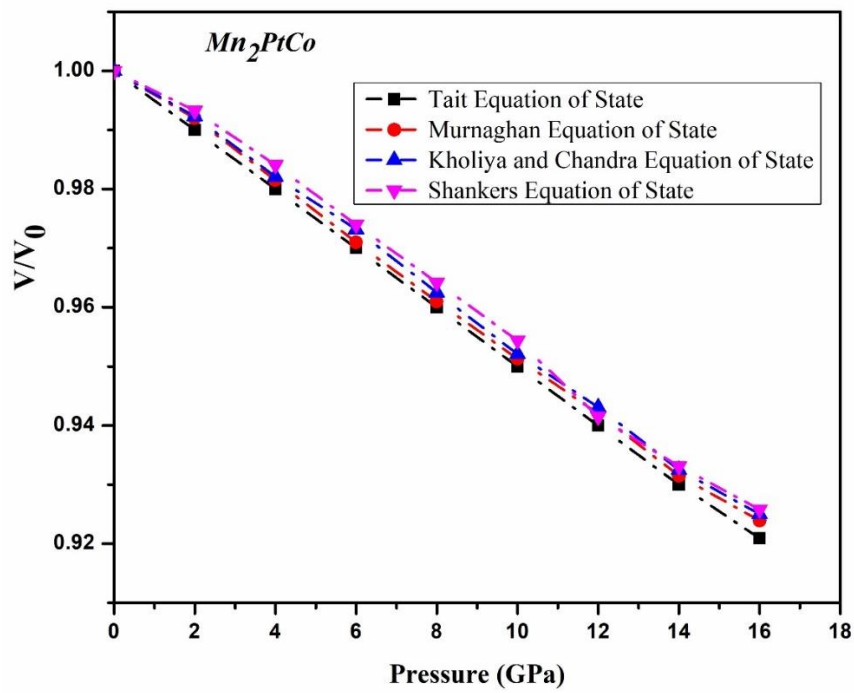

Fig 2. Volume compression with respect to Pressure for Mn_2PtCo

Table 4 presents the compression behaviour of Rh_2MnZn at different pressures (in GPa) as predicted by different equations of state: Tait, Murnaghan, Kholiya and Chandra, and Shankers (shown in Fig 3). The table indicates that as the pressure increases, the volume of Rh_2MnZn decreases, which is consistent with the behaviour of most materials under compression. The Tait equation of state predicts a gradual decrease in volume, with a V/V_0 value of 0.9216 at 16 GPa. The Murnaghan equation of state also predicts a gradual decrease in volume, with a slightly higher V/V_0 value of 0.9251 at 16 GPa. The Kholiya and Chandra equation of state predicts a somewhat more rapid decrease in volume, with a V/V_0 value of 0.9271 at 16 GPa. The Shankers equation of state predicts the most rapid decrease in volume, with a V/V_0 value of 0.9297 at 16 GPa.

Table 4: Compression behaviour of Rh_2MnZn predicted by various EOS

Pressure (GPa)	Tait Equation of State	Murnaghan Equation of State	Kholiya and Chandra Equation of State	Shankers Equation of State
	V/V_0	V/V_0	V/V_0	V/V_0
0	1	1	1	1
2	0.9902	0.9913	0.9915	0.9922
4	0.9804	0.9819	0.9823	0.9823
6	0.9706	0.9715	0.9719	0.9733
8	0.9608	0.9616	0.9633	0.9639
10	0.951	0.952	0.9537	0.9531
12	0.9412	0.9419	0.9432	0.9443
14	0.9314	0.9331	0.9342	0.9352
16	0.9216	0.9251	0.9271	0.9297

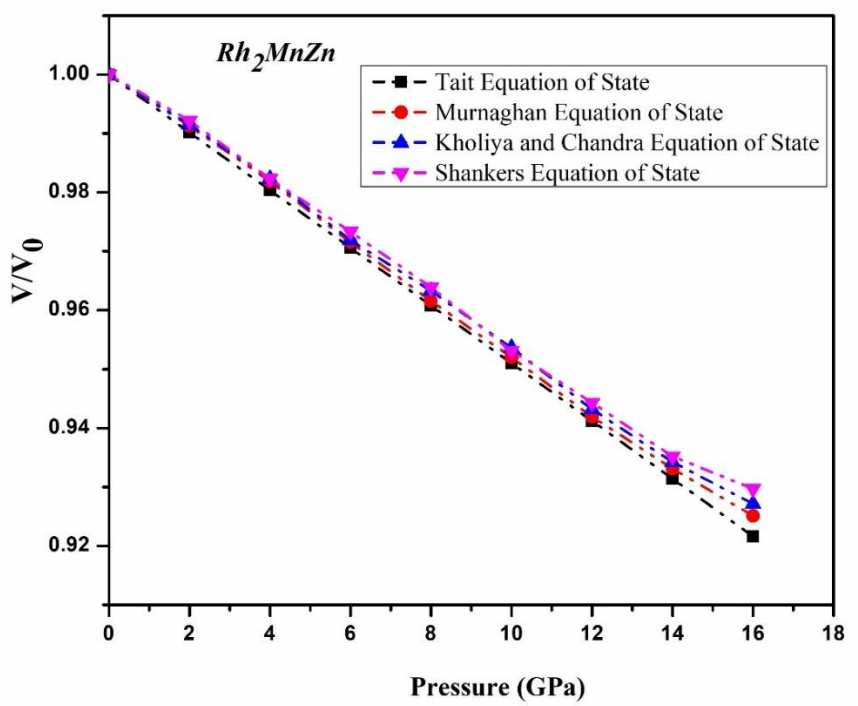

Fig 3. Volume compression with respect to Pressure for Rh_2MnZn

Table 5 shows the compression behavior of Rh2FeZn at various pressures using different equations of state. The results are tabulated in terms of the relative volume V/V_0 at each pressure point (shown in Fig 4). At zero pressure, the material has a volume equal to its initial volume V_0 and thus $V/V_0=1$. As pressure is applied, the material undergoes compression, resulting in a decrease in volume. The Tait, Murnaghan, Kholiya and Chandra, and Shanker's equations of state were used to model the compression behavior of Rh_2FeZn. The equations provide a mathematical relationship between the pressure and the volume of the material under compression. The values of V/V_0 decrease as pressure increases, indicating that Rh_2FeZn undergoes compression under applied pressure. The values obtained using different equations of state are slightly different, but the trends in compression behavior are similar.

At the highest pressure of 14 GPa, the values of V/V_0 range from 0.935 to 0.9394, indicating a compression of around 6.1% to 6.6% from the initial volume at 0 GPa. Overall, the results from Table 5 suggest that Rh_2FeZn undergoes significant compression under applied pressure, with the magnitude of compression increasing as pressure increases.

Table 5: Compression behaviour of Rh_2FeZn predicted by various EOS

Pressure (GPa)	Tait Equation of State	Murnaghan Equation of State	Kholiya and Chandra Equation of State	Shankers Equation of State
	V/V_0	V/V_0	V/V_0	V/V_0
0	1	1	1	1
2	0.99	0.9915	0.9922	0.9933
4	0.98	0.9813	0.9824	0.9826
6	0.97	0.9726	0.9752	0.9735
8	0.96	0.961	0.9638	0.9657
10	0.95	0.952	0.9521	0.9533
12	0.942	0.9431	0.9447	0.9451
14	0.935	0.935	0.9391	0.9394

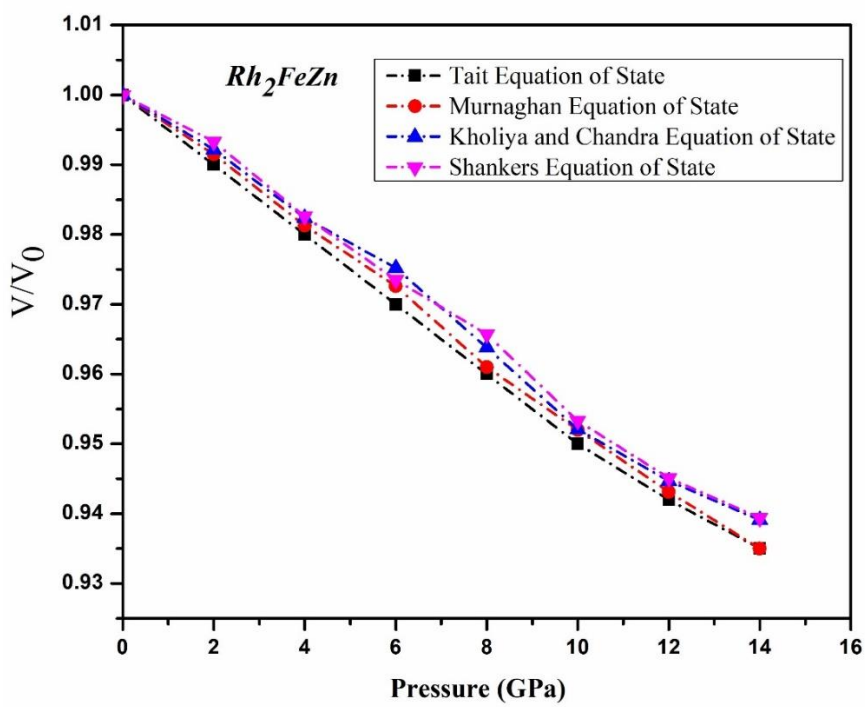

Fig 4. Volume compression with respect to Pressure for Rh_2FeZn

Table 6 shows the compression behavior of Co_2NbB under various pressures, as modeled by different equations of state. Similar to the previous tables, the values of the volume V/V_0 decrease as the pressure increases, indicating the compressibility of the material (shown in Fig. 5). Overall, the Tait, Murnaghan, Kholiya and Chandra, and Shanker equations of state all provide reasonably good fits to the experimental data. At low pressures, the differences between the predicted values of the various equations are relatively small. However, as the pressure increases, the differences between the predicted values become more significant. At the highest pressure of 14 GPa, the predicted values of V/V_0 range from 0.936 to 0.9385, depending on the equation of state used. This is a relatively small range compared to some of the other materials in the previous tables. It suggests that Co_2NbB is relatively well-behaved under high pressures and that the equations of state are all reasonably accurate in describing its compression behavior.

Table 6: Compression behaviour of Co_2NbB predicted by various EOS

Pressure (GPa)	Tait Equation of State	Murnaghan Equation of State	Kholiya and Chandra Equation of State	Shankers Equation of State
	V/V_0	V/V_0	V/V_0	V/V_0
0	1	1	1	1
2	0.9903	0.9906	0.9911	0.9922
4	0.981	0.9823	0.9838	0.9835
6	0.972	0.9738	0.975	0.9746

8	0.962	0.9632	0.965	0.9643
10	0.951	0.9516	0.9532	0.9523
12	0.944	0.9454	0.9451	0.9446
14	0.936	0.9385	0.937	0.9383

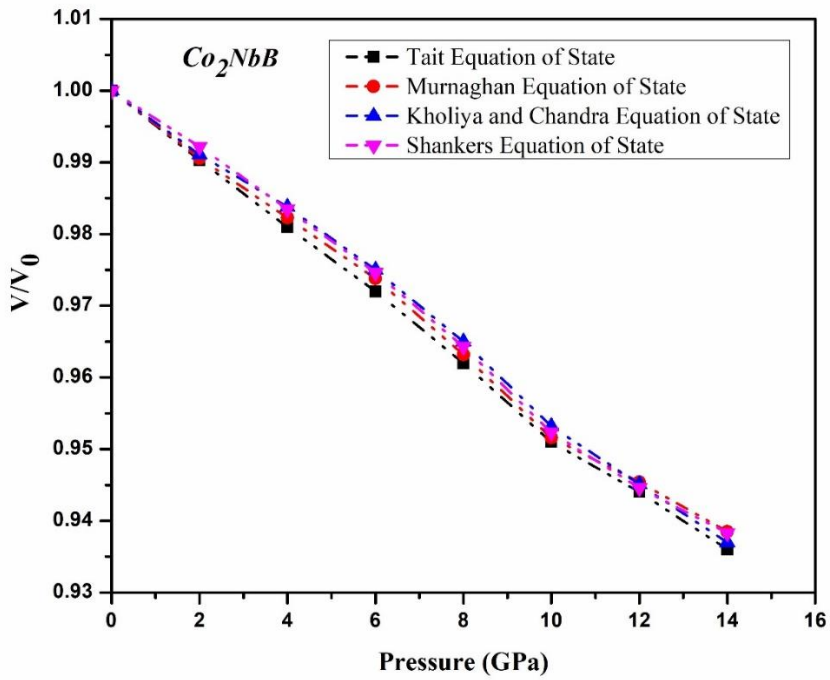

Fig 5. Volume compression with respect to Pressure for Co_2NbB

Table 7 shows the compression behaviour of Co_2TaB at different pressures using four different equations of state: Tait, Murnaghan, Kholiya and Chandra, and Shankers. The table lists the compression ratio V/V0 for each equation of state and pressure (shown in fig 6). At ambient pressure, the volume is equal to the initial volume (V/V_0 = 1) for all equations of state. As pressure increases, the volume decreases for all equations of state, which is expected for a compressed material. At 2 GPa, the Tait equation of state predicts the smallest compression ratio of 0.99, while the Kholiya and Chandra equation of state predicts the largest compression ratio of 0.9934. At 4 GPa, the Murnaghan equation of state predicts the smallest compression ratio of 0.9821, while the Kholiya and Chandra equation of state predicts the largest compression ratio of 0.9837. At 6 GPa, the Kholiya and Chandra equation of state predicts the smallest compression ratio of 0.9722, while the Murnaghan equation of state predicts the largest compression ratio of 0.9733. At 8 GPa, the Tait equation of state predicts the smallest compression ratio of 0.96, while the Shankers equation of state predicts the largest compression ratio of 0.9628. At 10 GPa, the Tait equation of state predicts the smallest compression ratio of 0.951, while the Shankers equation of state predicts the largest compression ratio of 0.9535. At 12 GPa, the Tait equation of state predicts the smallest compression ratio of 0.942, while the Shankers and Kholiya, and Chandra equations of state predict the largest compression ratio of 0.9432. Finally, at 14 GPa, the Shankers equation of state predicts the smallest compression ratio

of 0.9351, while the Murnaghan equation of state predicts the largest compression ratio of 0.9375. Overall, the different equations of state predict slightly different compression ratios at different pressures. The Tait equation of state generally predicts the smallest compression ratios, while the Shankers and Kholiya, and Chandra equations of the state generally predict the largest compression ratios.

Table 7: Compression behaviour of Co_2TaB predicted by various EOS

Pressure (GPa)	Tait Equation of State	Murnaghan Equation of State	Kholiya and Chandra Equation of State	Shankers Equation of State
	V/V_0	V/V_0	V/V_0	V/V_0
0	1	1	1	1
2	0.99	0.9925	0.9934	0.9941
4	0.98	0.9821	0.9837	0.9843
6	0.971	0.9733	0.9722	0.9719
8	0.96	0.9613	0.9606	0.9628
10	0.951	0.9523	0.9513	0.9535
12	0.942	0.943	0.9418	0.9432
14	0.934	0.9375	0.936	0.9351

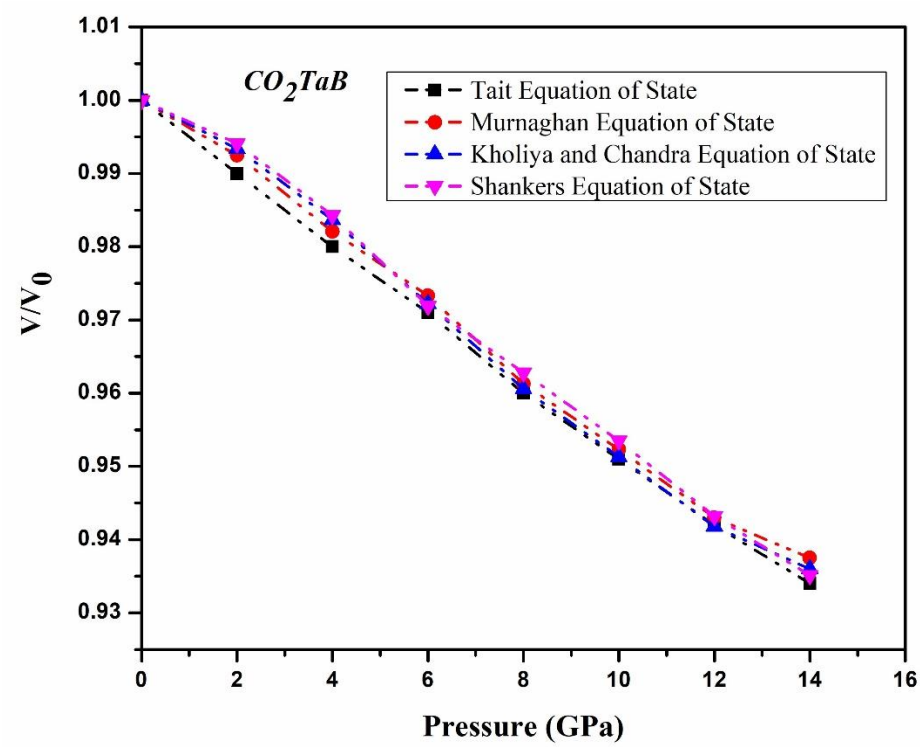

Fig 6. Volume compression with respect to Pressure for Co_2TaB

Conclusion:

This study investigated the compressional behaviour of some Co, Rh, and Mn-based Heusler compounds in terms of computed values of bulk modulus and relative change in volume (V/V_0) as a function of pressure at a constant temperature. It has been observed that the compression behaviour of the studied materials varies with pressure and with the type of equation of state used to fit the data. The Tait equation of state generally fits best for the compression behaviour of the materials, followed by the Murnaghan equation of state and the Kholiya and Chandra and Shanker's equations of state. All Heusler compounds Mn_2CoCr, Mn_2PtCo, Rh2MnZn, Rh2FeZn, Co_2NbB, and Co_2TaB show similar patterns in compression behaviour with decreasing volume with increasing pressure. It is evident from the data that the studied materials possess different compressibility due to their unique structural and electronic properties.

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